Scattering of light by large nonspherical particles: ray-tracing approximation versus T-matrix method

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We report, for the first time to our knowledge, comparisons of light-scattering computations for large, randomly oriented, moderately absorbing spheroids based on the geometric-optics approximation and the exact T-matrix method. We show that in most cases the geometric-optics approximation is (much) more accurate for spheroids than for surface-equivalent spheres and can be used in phase function computations (but not in polarization computations) for nonspherical particles with size parameters as small as 60. Differences in the single-scattering albedo between geometric-optics and T-matrix results are surprisingly small, even for small size parameters. © 1995 Optical Society of America

Ray-tracing techniques based on the geometric-optics approximation[1] (GO) are widely used in atmospheric optics to compute scattering properties of nonspherical particles. In principle, the GO becomes accurate only in the limit $d/\lambda \to \infty$, where d is the smallest dimension of the scattering particle and λ is the wavelength of the incident radiation. However, the GO is often applied to particles with moderate size parameters, in which case it can result in large and *a priori* unknown errors. Therefore it is important to ascertain the domain of applicability of GO by comparison of ray-tracing computations with results obtained by exact methods. Because exact light-scattering computations for nonspherical particles used to be extremely difficult and time consuming, so far the GO has been examined only versus Mie calculations for perfect spheres.[2] However, recently the exact T-matrix method[3] (TM) has been substantially improved[4] and has become applicable to rotationally symmetric particles with size parameters greatly exceeding 50.[5] Therefore it is our aim in this Letter to compare, for the first time to our knowledge, approximate ray-tracing computations for randomly oriented spheroids with accurate TM computations. Most of our results have been computed for the index of refraction $1.394 + 0.00684i$ corresponding to pure water ice at $\lambda = 3.732 \ \mu$m.[6] This choice was motivated by our interest in the transfer of infrared solar radiation in cirrus clouds, in which case scattering particles are distinctly nonspherical and often have size parameters less than 100.[7] Although cirrus cloud particles are not spheroids, our goal is to examine the general effect of particle nonsphericity on the performance of the ray-tracing approximation. Furthermore, the often observed random shapes of real ice particles give rise to a relatively smooth angular dependence of their scattering properties, which may well be similar to that of spheroids.

In ray-tracing computations an incident plane electromagnetic wave is simulated by a sufficiently large number of parallel rays. Each individual ray is traced for a given particle geometry by Snell's law and Fresnel's equations.[8] The sampling of all escaping light rays into predefined angular bins supplemented by the computation of diffraction of the incident plane wave on the particle projection yields a quantitative image of the particle-scattering properties. The effect of the nonzero imaginary part of the refractive index is taken into account by modification of Snell's law, as described in Ref. 8. A detailed discussion of the GO can be found in Refs. 9 and 10. The T-matrix method is described in Refs. 3–5 and is not discussed here.

Following Ref. 2, we first checked our ray-tracing code by comparing geometric-optics calculations for big spheres with rigorous Mie computations. We were able to reproduce the comparison examples given in Ref. 2 and found an excellent agreement between ray-tracing and Mie computations, provided that the sphere size parameter was sufficiently large.

Below we report GO and TM computations for randomly oriented prolate and oblate spheroids with an aspect ratio (ratio of the largest to the smallest spheroidal axes) of 2 and compare them with GO and Mie computations for surface-equivalent spheres. Because GO computations of the scattering phase function and the degree of linear polarization are mean values for predefined angular bins, all TM and Mie

calculations were performed for a large number of scattering angles and then averaged over the same GO bins. GO and TM computations for spheroids pertain to monodisperse particles, whereas Mie and GO results for spheres were averaged over a size distribution with an effective variance (as defined in Ref. 2) of 0.1 in order to smooth out oscillations that are due to interference and diffraction effects. For randomly oriented spheroids, size averaging was found to be unnecessary because of the smoothing effect of averaging over orientations.

Figures 1 and 2 show the scattering phase function and the degree of linear polarization for unpolarized incident light[2] versus the scattering angle for prolate spheroids and surface-equivalent spheres. For spheroids $x = 2\pi r_{es}/\lambda$ is the size parameter of the equal-surface-area sphere, whereas for spheres x is the effective size parameter of the size distribution.[2] It is seen that for a size parameter of 60, GO and TM spheroidal phase functions agree fairly well over the entire range of scattering angles. In contrast, GO and Mie computations of the phase function for spheres exhibit much stronger differences, especially in the backscattering region, where GO completely fails to reproduce the strong glory feature. Thus it appears that particle nonsphericity tends to make the GO more accurate and applicable to smaller particles. The small intensity maximum at approximately 80° scattering angle for spheroids corresponds to the primary rainbow at 144° in the spherical phase function. This rainbow feature moves toward smaller scattering angles as the particle aspect ratio departs from 1. Note that increasing size parameter also implies increasing absorption inside the particle. This causes the GO results to exhibit increasingly strong rainbow features, including the secondary rainbow for spheres at 114°, as the size parameter decreases. This also means that the accuracy of GO computations for a given size parameter should deteriorate with decreasing absorption. Our computations for smaller imaginary refractive indices have shown that this is indeed the case.

Figure 2 demonstrates that the overall differences between the GO and TM spheroidal polarization curves are considerably smaller than those between the GO and Mie polarization results for spheres, especially for a size parameter of 60. However, GO/TM polarization differences are still significant even for this fairly large size parameter and are much more pronounced than those in the GO and TM spheroidal phase functions. From the GO standpoint, the angular dependence of linear polarization is determined by positively polarizing external reflections with a maximum at the Brewster angle, weakly polarizing direct transmissions, and positively polarizing internal reflections. External reflections cause the positive polarization peak for GO computations. Positively polarizing rainbow rays result in a rise of linear polarization at the rainbow angles. To some extent, these GO features are also seen in the exact Mie and TM results. The present ray-tracing technique does not take into account interference of different rays leaving the particle. We expect that taking the effect of interference into account can bring the GO results in closer agreement with exact computations.

A similar comparison was performed for randomly oriented oblate spheroids with size parameters varying from 10 to 80. Again, it was found that ray tracing is more accurate for spheroidal than for surface-equivalent spherical particles and gives accurate enough phase functions for spheroids with size parameters larger than approximately 60.

Figure 3 shows that GO computations of the asymmetry parameter of the phase function g converge
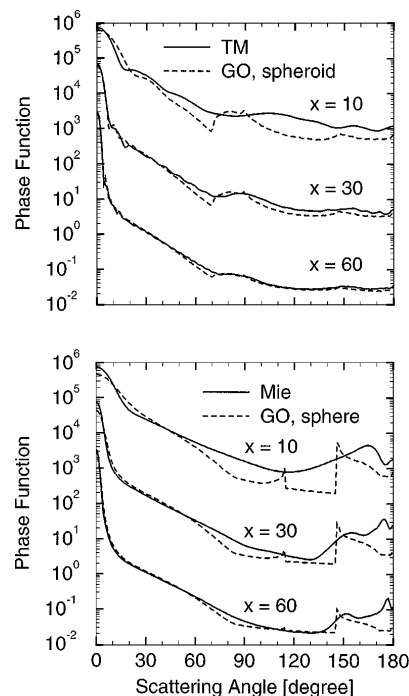

Fig. 1. Phase function versus scattering angle for spheres and randomly oriented prolate spheroids. The phase functions for size parameters 30 and 10 are multiplied by 10^2 and 10^4, respectively.
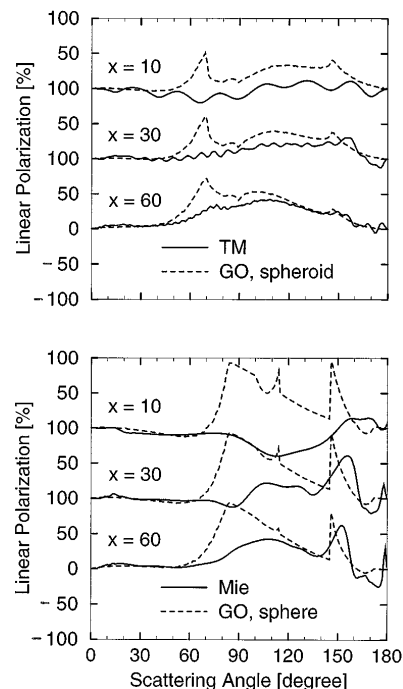

Fig. 2. Degree of linear polarization versus scattering angle for spheres and randomly oriented prolate spheroids.
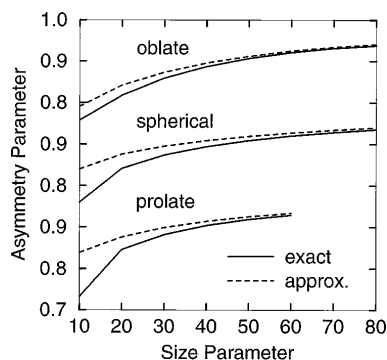
Fig. 3. Asymmetry parameter of the phase function versus size parameter for spheres and randomly oriented prolate and oblate spheroids.

Table 1. Single-Scattering Albedo versus Size Parameter for Spheres and Randomly Oriented Prolate and Oblate Spheroids[a]

x	Prolate	Δ(GO)	Sphere	Δ(GO)	Oblate	Δ(GO)
10	0.886	−1.0	0.900	0.9	0.889	−0.9
20	0.804	−1.7	0.817	0.5	0.803	−1.9
30	0.754	−0.8	0.749	−0.7	0.748	−1.3
40	0.713	−0.5	0.707	−0.6	0.705	−0.8
50	0.680	−0.4	0.676	−0.3	0.672	−0.3
60	0.654	−0.3	0.652	0.0	0.646	0.1
70			0.630	−0.2	0.625	0.5
80			0.614	−0.1	0.609	0.7

[a]GO results are given as percentage differences of Mie and TM results.

to the exact results as the particle size parameter increases. Note that the GO always overestimates g, apparently because interference of different rays leaving the particle is not taken into account. Importantly, the g values for spheroids converge to the exact computations faster than those for surface-equivalent spheres, which corroborates our conclusion that nonsphericity makes the GO applicable to smaller particles.

Finally, Table 1 compares approximate and exact computations of the single-scattering albedo. Strikingly, in almost all cases GO gives fairly good accuracy, even for the smallest size parameter. This suggests that the GO concept of energy attenuation along internal ray paths can work surprisingly well.

In conclusion, that the exact TM and approximate GO computations of the scattering phase function for moderately absorbing randomly oriented spheroids essentially coincide at size parameters larger than approximately 60 renders possible a complete size parameter coverage by a combination of these two techniques. Also we note that although in this Letter we have shown and discussed only computations for the refractive index $1.394 + 0.00684i$, our conclusions are fully corroborated by similar computations for the refractive index $1.5 + 0.01i$ representing dustlike tropospheric aerosols at visible wavelengths.[11] Of course our results must be further substantiated by computations for other refractive indices, eccentricities, and shapes, including nonrotationally symmetric particles.

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